

N,N-Dimethylformamide
68-12-2 | DTXSID6020515

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.11×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.26×10^{-1}

Confidence level: 6.93×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Formic acid, propyl ester

Measured: 2.38×10^{-12}

Predicted: 1.78×10^{-12}

Image not found

Ethyl formate

Measured: 1.02×10^{-12}

Predicted: 1.05×10^{-12}

Image not found

tert-Butyl formate

Measured: 7.37×10^{-13}

Predicted: 1.01×10^{-12}

Image not found

Formic acid, butyl ester

Measured: 3.12×10^{-12}

Predicted: 2.12×10^{-12}

Image not found

Methyl formate

Measured: 2.27×10^{-13}

Predicted: 3.44×10^{-13}